

Ground state properties of a Tonks-Girardeau Gas in a periodic potential

Bo-Bo Wei, Shi-Jian Gu, and Hai-Qing Lin

*Department of Physics and Institute of Theoretical Physics,
The Chinese University of Hong Kong, Hong Kong, China*

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In this paper, we investigate the ground-state properties of a bosonic Tonks-Girardeau gas confined in a one-dimensional periodic potential. The single-particle reduced-density matrix is computed numerically for systems up to $N = 41$ bosons. Then we are able to study the scaling behavior of the occupation numbers of the most dominant orbital for both commensurate and non-commensurate cases, which correspond to an insulating phase and a conducting phase, respectively. We find that, in the commensurate case, the fractional occupation decays as $f_0 \propto 1/\ln N$ with the particle number, while $f_0 \propto 1/N^{0.44}$ in the non-commensurate case. So there is no BEC in both cases. The study of zero momentum peaks shows that $n(0) \propto N$ in commensurate case, which implies that all bosons are localized in the insulating phase.

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I. INTRODUCTION

With the development of optical lattices and atom chip traps, quasi-one-dimensional cold atom systems have been realized by tightly confining the particle's motion in two directions to zero-point oscillation [1, 2, 3]. Meanwhile, using the Feshbach resonance or by tuning of the effective mass of particles moving in a periodic potential [1, 4], the inter-particle scattering length can be tuned to almost any desired value. These progresses have led to experimental realizations of the one-dimensional (1D) exactly solvable model that describes an interacting Bose gas [5, 6, 7, 8].

At very low temperatures and densities, a 1D Bose gas is expected to behave as a gas of impenetrable particles known as hard-core bosons [9, 10, 11]. In particular, two recent experiments successfully achieved the required so-called Tonks-Girardeau (TG) regime and made the TG gas a physical reality [1, 2]. Physically, a TG gas is defined to be a 1D strongly correlated quantum gas consisting of bosons with hardcore interaction. This model of a 1D gas was first proposed by Tonks in 1936 [12]. As a milestone development to the model, Girardeau solved the model exactly by the famous Bose-Fermi mapping theorem [5, 8, 13], where the TG gas can be mapped to a spinless free fermion gas. Recently, it was found that the above case is just a special case of a general mapping theorem between bosons and fermions in one dimension, where the particles can interact with finite strength [14, 15].

Since the TG gas is both theoretical exactly solvable and experimental accessible, there are great research interest recently in the TG gas in different trapping potentials [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32]. A review on relevant studies in this interesting subject can be found in a recent article by Yukalov and Girardeau [13]. In particular, Lin and Wu investigated the ground-state properties of a TG in periodic potentials [28]. They used the Monte Carlo integration technique to compute the single-particle reduced

density matrix (SPRDM) for small systems up to $N = 7$ bosons. Their analysis of ground states shows that when the number of bosons N is commensurate with the number of wells M in the periodic potential, the boson system is a Mott insulator whose energy gap, however, is given by the single-particle band gap of the periodic potential; when N is not commensurate with M , the system is a metal (not a superfluid). The purpose of this work is to compute the SPRDM for large systems containing more than 40 particles, and then study scaling relations, quantitative predictions for scaling exponents of the ground-state occupation numbers, and zero-momentum peak in different filling conditions. Therefore we put particular emphasis on examining the ground-state fractional occupation in these two phases of the system.

The remaining of this paper is organized as follows. In Sec. II, we introduce the model Hamiltonian of the system and describe the single-particle eigenstates and eigenvalues which will be used. In Sec. III, we review the Bose-Fermi mapping theorem and then construct the exact many-body ground state wave function. In Sec. IV, we devote ourselves to study the many-body properties of the TG gas. Summary and conclusion are given in Sec. V.

II. MODEL HAMILTONIAN AND SINGLE-PARTICLE EIGENSTATES

A. Model Hamiltonian

We consider a gas of N hardcore bosons trapped in a tight atomic waveguide. The waveguide restricts strongly the dynamics of the gas in the transversal directions, such that in the low temperature limit we can define our model in the longitudinal direction only. In this direction we consider a periodic potential such that the many-particle

Hamiltonian at low density can be written as

$$H = \sum_{j=1}^N \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + V(x_j) \right], \quad (1)$$

where m is the mass of a single boson, $V(x) = V(x + d)$ the periodic potential with d being the period. In this work, we use the Kronig-Penney (KP) potential as a candidate for the periodic potential, which takes the form

$$V(x) = \gamma \sum_{j=1}^M \delta(x - jd) \quad (2)$$

where γ is the strength of the δ potential and M is the total number of wells.

B. Eigenstates and eigenvalues of periodic potential

We impose the usual periodic boundary conditions and use d as the unit of distance and $\hbar^2/(2m)$ as the unit of energy. Then we arrive at the following dimensionless single-particle Hamiltonian,

$$H = -\frac{\partial^2}{\partial x^2} + \gamma \sum_{j=1}^M \delta(x - jd). \quad (3)$$

The Hamiltonian can be exactly solved. One can find the solution in any standard textbook of solid state physics. We review the result again for later computation. The Bloch wave functions take the form

$$\begin{aligned} \psi_\alpha(x) &= C_\alpha [\sin(k_\alpha x) + e^{-iK_\alpha} \sin[k_\alpha(1-x)]], 0 \leq x \leq 1, \\ \psi_\alpha(x) &= e^{iK_\alpha[x]} \psi_\alpha(x - [x]), 1 \leq x \leq M. \end{aligned} \quad (4)$$

The eigenenergy is

$$E_\alpha = k_\alpha^2 \quad (5)$$

where k_α satisfies the transcendental equation

$$\cos(k_\alpha) + \gamma \frac{\sin(k_\alpha)}{2k_\alpha} = \cos(K_\alpha), \quad (6)$$

$$K_\alpha = \frac{2\pi\alpha}{M}, \quad \alpha = 0, \pm 1 \pm 2, \dots \pm \frac{M-1}{2} \quad (7)$$

and the normalization constant for the Bloch wave function is given by

$$C_\alpha = \sqrt{\frac{k_\alpha}{M(k_\alpha - \frac{1}{2} \sin(2k_\alpha) + \cos K_\alpha (\sin k_\alpha - k_\alpha \cos k_\alpha))}}. \quad (8)$$

III. BOSE-FERMI MAPPING THEOREM AND MANY-BODY WAVE FUNCTIONS OF THE TG GAS

For a system of N identical hardcore bosons in the 1D external potential $V(x)$, the bosons interact with each other by impenetrable pointlike interactions, which can be more conveniently treated as a boundary condition for the many-body wave function $\Psi_B(x_1, x_2, \dots, x_N, t)$:

$$\Psi_B(x_1, x_2, \dots, x_N, t) = 0 \text{ if } x_i = x_j, 1 \leq i < j \leq N. \quad (9)$$

Then the hardcore boson gas can be considered as a free boson gas governed by the following free Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \Psi_B = \sum_{j=1}^N \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + V(x_j) \right] \Psi_B, \quad (10)$$

where the wave function Ψ_B satisfies the hardcore boundary condition of Eq. (9). Based on the observation that the hardcore boundary condition of Eq. (9) is automatically satisfied by a wave function of fermions due to its antisymmetry, Girardeau [5, 8] gave the exact many-body wave function of the hardcore boson system via the famous Bose-Fermi mapping, which relates the wave function of hardcore bosons to that of noninteracting spinless fermions in the same trapping potential:

$$\Psi_B(x_1, x_2, \dots, x_N) = A \Psi_F(x_1, x_2, \dots, x_N, t). \quad (11)$$

with

$$A = \prod_{1 \leq i < j \leq N} \text{sgn}(x_i - x_j), \quad (12)$$

where sgn is sign function and A is unit antisymmetric function which ensures that Ψ_B has proper symmetry under the exchange of two bosons. The free fermionic wave function can be compactly written in form of the Slater determinant

$$\Psi_F = \frac{1}{\sqrt{N!}} \text{Det}_{m,j=1}^N [\psi_m(x_j, t)]. \quad (13)$$

where $\psi_m, m = 1, \dots, N$ is single-particle eigenstate. The eigenstates are governed by a set of uncoupled single-particle Schrödinger equations,

$$i\hbar \frac{\partial}{\partial t} \psi_m(x) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi_m(x). \quad (14)$$

Eqs. (11), (13) and (14) describe how to construct the exact many-body wave functions of a TG gas in any external potential $V(x)$. Then the wave function of the TG gas is

$$\Psi_B = A(x_1, x_2, \dots, x_N) \frac{1}{\sqrt{N!}} \text{Det}_{m,j=1}^N [\psi_m(x_j, t)]. \quad (15)$$

where $\psi_m(x)$ is the single-particle eigenstate in the potential $V(x)$.

For the periodic potential that we are interested in, the single-particle eigen function is given by Eq. (4), then we can construct the exact many-body wave function of the TG gas in the KP potential according to the above procedures. The ground-state many-body properties of the TG gas in the KP potential can be studied from this exact wave function.

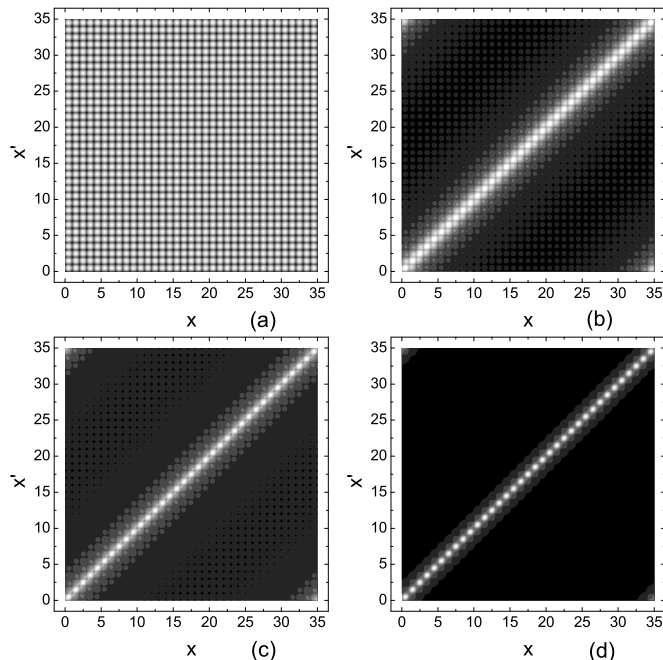


FIG. 1: Single-particle reduced density matrix, $\rho(x, x')$, of the TG gas in periodic potential for different particle numbers, (a) $N = 1$, (b) $N = 15$, (c) $N = 25$, (d) $N = 35$ when number of wells $M = 35$.

IV. MANY-BODY PROPERTIES OF TG GAS IN PERIODIC POTENTIALS

In this section we numerically evaluate the ground-state properties of the 1D TG gas in the periodic potential using the exact many-body wave function of the previous section.

A. Single-particle reduced density matrix

The many-body wave function Ψ_B fully describes the state of the system. However, its form does not transparently yield physical information related to many important observable such as occupation numbers of natural orbital and the momentum distribution. The expectation value of one-body observable are readily obtained

from the SPRDM,

$$\rho(x, x') = N \int dx_2 \cdots x_N \Psi_B^*(x, x_2, \dots, x_N) \times \Psi_B(x', x_2, \dots, x_N), \quad (16)$$

which satisfies the normalization condition

$$\int \rho(x, x) dx = N \quad (17)$$

Although the exact many-body wave function of the TG gas can be written in a compact form, the calculation of the SPRDM is a very difficult task as it is very time consuming to calculate multidimensional integrals in SPRDM for a large system [18, 19, 20, 21, 22, 23, 24, 25, 33, 34]. However, in the TG limit the SPRDM can be written in a matrix product form in terms of single-particle eigenstates [29]

$$\rho(x, x') = \sum_{i,j=1}^N \psi_i^*(x) A_{ij}(x, x') \psi_j(x'). \quad (18)$$

Here the $N \times N$ matrix $\mathbf{A}(x, x') = \{A_{ij}(x, x')\}$ takes the form,

$$\mathbf{A} = (\mathbf{P}^{-1})^T \text{Det } \mathbf{P} \quad (19)$$

where the entries of the matrix \mathbf{P} are $P_{ij}(x, x') = \delta_{i,j} - 2 \int_x^{x'} \psi_i^*(t) \psi_j(t) dt$, and we can assume $x < x'$ without loss of generality. This formalism of the SPRDM enables us to calculate considerable large systems of the TG gas.

The SPRDM expresses self-correlation and one can view $\rho(x, x')$ as the probability that, having detected the particle at position x , a second measurement, immediately following the first, will find the particle at the point x' . Classically, $\rho(x, x') = \delta(x - x')$, so the off diagonal elements of SPRDM comes from purely quantum correlations of the particles. Fig. 1 displays contour plots of SPRDM, $\rho(x, x')$, for the number of particle $N = 1, 15, 25$ and 35 respectively, where the number of wells of the periodic potential $M = 35$. We clearly see a characteristic pattern for each value of N : The SPRDM are largest close to the diagonal elements which stands for the position density distributions. The diagonal elements of SPRDM shows oscillations due to the barrier of the periodic potential which tends to repel the particles and push the particles stay inside the well. The off-diagonal elements of the SPRDM relate to off-diagonal long range order (ODLRO) [36] and we can see that the off-diagonal elements are decreasing in contrast to the diagonal as the number of particles N increases. It means that the repulsive interaction tends to destroy the ODLRO, and ODLRO vanishes for a system of hard core bosons in a 1D periodic potentials in the thermodynamic limit. As $N = M$, the SPRDM is almost localized, and the system becomes an insulator.

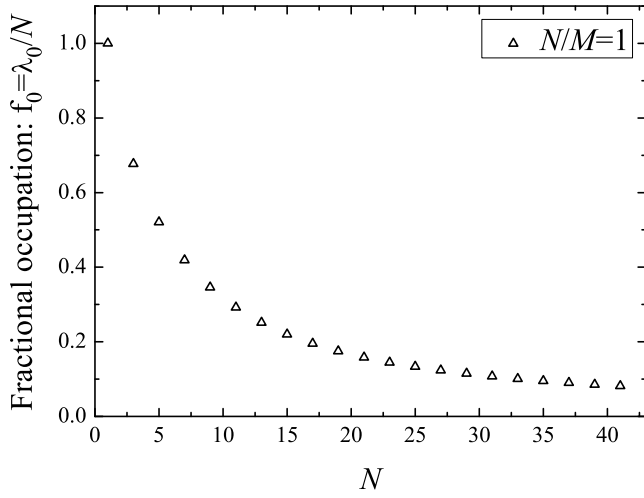


FIG. 2: Fractional occupations, $f_0 = \lambda_0/N$, as a function of particle number N at commensurate case, $N/M = 1$, when periodic potential strength $\gamma = 2$.

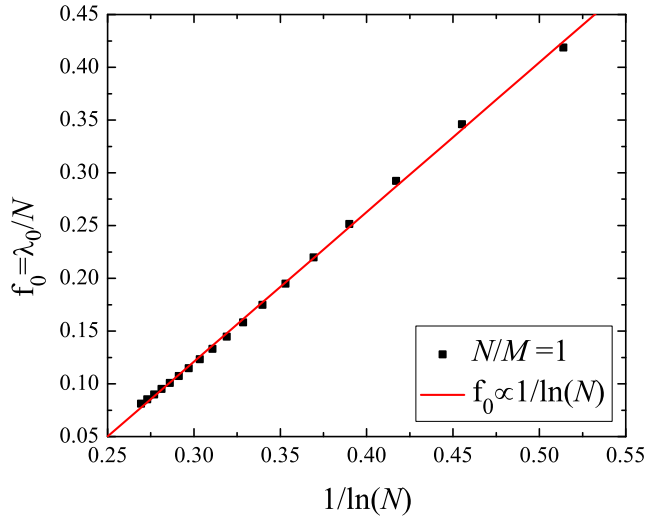


FIG. 3: Occupation numbers of lowest orbital λ_0 , as a function of particle number, $1/\ln(N)$, at commensurate case, $N/M = 1$, when periodic potential strength $\gamma = 2$.

B. Occupation numbers and natural orbital

In a macroscopic system, the presence or absence of BEC is determined by the behavior of $\rho(x, x')$ as $x - x'$. ODLRO is present if the largest eigenvalue of $\rho(x, x')$ is macroscopically non-vanishing. In this case the system exhibits BEC and the corresponding eigenfunction, the condensate orbital, plays the role of an order parameter [35, 36]. The fraction of particles that are in the lowest orbital is related to the largest eigenvalue of the SPRDM by $f_0 = \lambda_0/N$. Therefore, in analogy to the macroscopic occupation of a single eigenstate in a Bose-Einstein condensate, this orbital is sometimes referred

to as the “BEC” state and the quantity hence acts as a measure of the coherence in the system.

The occupation numbers of the natural orbital are defined as eigenvalues of the SPRDM,

$$\int dx' \rho(x, x') \phi_i(x') = \lambda_i \phi_i(x), i = 0, 1, \dots, \quad (20)$$

where $\phi_i(x)$ are the so called natural orbitals, which are obtained from the eigenfunctions of the SPRDM and it represents an effective single-particle state. The corresponding eigenvalue λ_i is occupation number of the i -th natural orbital and satisfies $\sum_i \lambda_i = N$. The SPRDM is diagonal in the natural orbital basis. The corresponding eigenvalue of each orbital gives the population probability of that orbital. The natural orbitals can be ordered according to their eigenvalues, we assume $\lambda_0 > \lambda_1 > \dots$ without loss of generality.

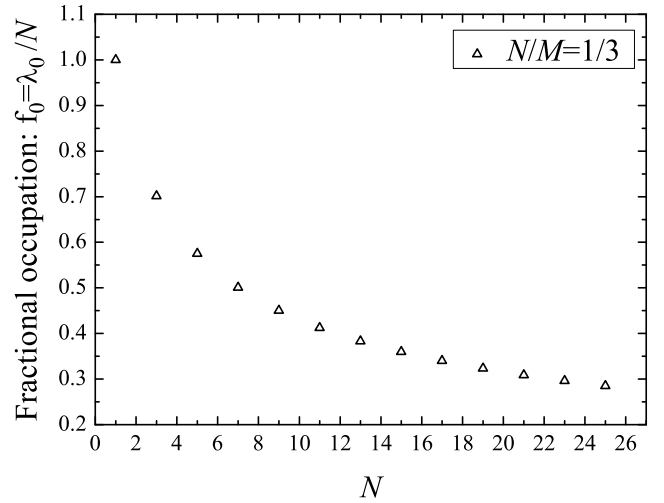


FIG. 4: Fractional occupations, $f_0 = \lambda_0/N$, as a function of particle number N , at non-commensurate case, $N/M = 1/3$, when periodic potential strength $\gamma = 2$.

The importance of natural orbitals is that, for a boson system, one can infer whether the system is a BEC state or not from scaling behavior of the occupation number of the lowest natural orbital λ_0 [35, 36]. The system will show a BEC behavior if the occupation number of the lowest natural orbital is proportional to the particle number of the system, which means a macroscopic number of particles will condensed to the lowest orbital. Then the corresponding natural orbital will be the eigenfunction of the BEC. For the TG gas in periodic potentials, there are two different phases in the ground state [28]: one is a Mott-insulator for the commensurate case where N/M is an integer. In this phase, one or more Bloch bands have been fully occupied. The other is a boson conductor phase for non-commensurate case where N/M is a fractional number. In this phase, the Bloch bands are partially occupied. What we are interested here is

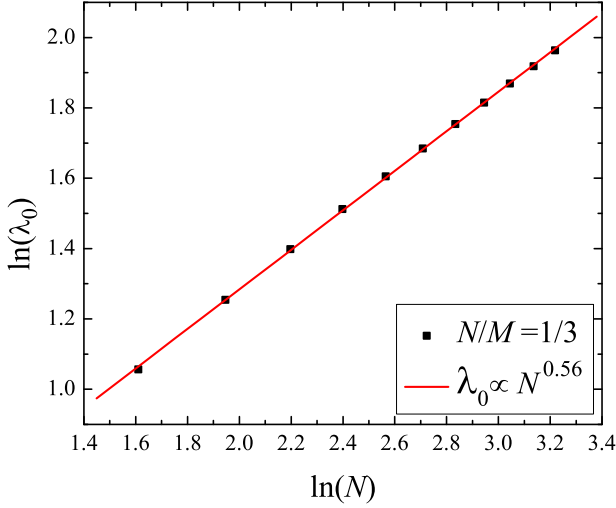


FIG. 5: Occupation numbers of lowest orbital $\ln(\lambda_0)$, as a function of particle number, $\ln(N)$, at non-commensurate case, $N/M = 1/3$, when periodic potential strength $\gamma = 2$.

the BEC probability and the scaling behavior of the occupation number of lowest orbital in different phases. Diagonalizing the SPRDM numerically, we can obtain the occupation number of lowest orbital for different particle numbers up to 41.

We have shown the fractional occupations of the lowest orbital, $f_0 = \lambda_0/N$, with particle numbers N , at commensurate case (the lowest Bloch band has been fully occupied) and $\gamma = 2$ in Fig. 2. From the figure, we can see that the fractional occupations of lowest orbital decrease with the particle number increases and it will vanish in the thermodynamic limit. By doing finite size scaling in Fig. 3, we found that the fractional occupation of lowest orbital decreases with the system sizes as $f_0 \propto 1/\ln(N)$ in the Mott-insulating phase and it vanishes in the thermodynamic limit. So we can infer that there is also no BEC for the commensurate case.

The fractional occupations of the lowest orbital, $f_0 = \lambda_0/N$, with particle numbers N , in non-commensurate case for $N/M = 1/3$ and $\gamma = 2$ is shown in Fig. 4. We can see that the fractional occupations of lowest orbital decrease with the particle number increases and will vanish in the thermodynamic limit. Doing finite size scaling of occupation number of lowest orbital in Fig. 5, from which we can find that the occupation numbers of lowest orbital λ_0 shows power law dependence on the particle number N of the system in non-commensurate case, i.e. $\lambda_0 \sim N^{0.56}$. So there is no BEC behavior also in the non-commensurate case.

C. Momentum density distribution

Although the position density profiles and energy are exactly the same between the hardcore boson gas and

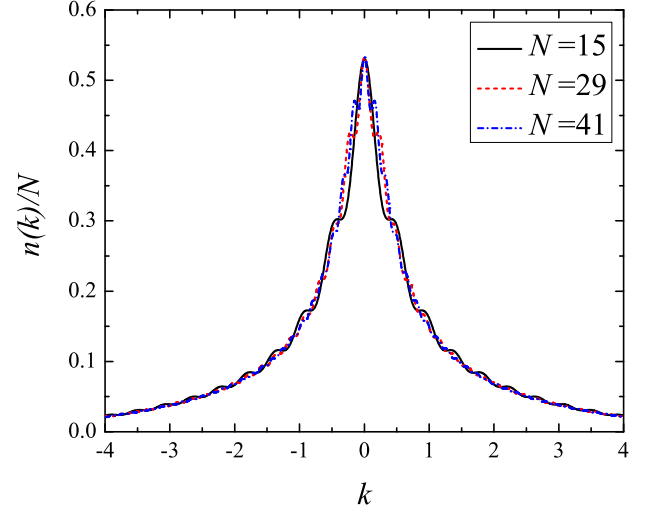


FIG. 6: Momentum distributions for several particle number at commensurate case, $N/M = 1$, when periodic potential strength $\gamma = 2$.

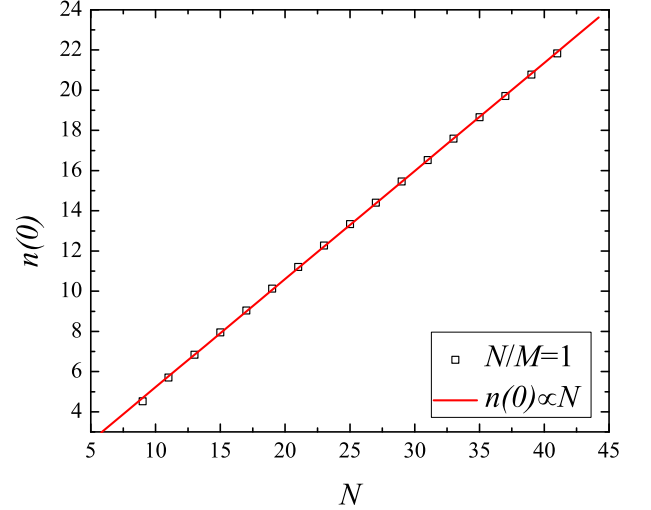


FIG. 7: $n(0)$, as a function of particle number N at commensurate case, $N/M = 1$, when periodic potential strength $\gamma = 2$.

their corresponding spinless fermion counterpart due to Bose-Fermi mapping theorem, the momentum distributions differ considerably from each other [28, 32]. The momentum distribution can be obtained from the SPRDM as

$$n(k) = 2\pi^{-1} \int dx dx' \rho(x, x') e^{-ik(x-x')}. \quad (21)$$

The momentum distributions of the TG gas in the commensurate case are shown in Fig. 6 for various particle numbers. We can see that the momentum distributions of the TG gas has a bosonic structure, which has peaks at $k = 0$ and the profiles are narrow. Although a TG gas

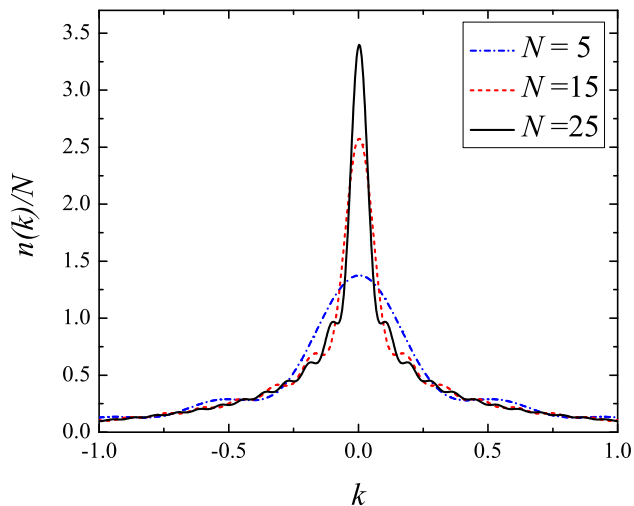


FIG. 8: Momentum distributions for several particle number at non-commensurate case, $N/M = 1/3$, when periodic potential strength $\gamma = 2$.

has the same energy spectrum and position profiles with its fermionic counterpart, their momentum distributions are very different. In addition, the profiles of momentum distributions is nearly unchanged with the particle number increases at commensurate case. This is because in the Mott-insulating phase the particles are localized in the real space. The oscillations in the momentum distribution comes from the finite size effect, it will vanish in thermodynamic limit. What is more interesting here is that we find the momentum distributions have same zero momentum peaks after rescale. Then we plot $n(0)$ as a function of particle number in Fig. 7. It clearly shows that $n(0) \propto N$ in the commensurate case. Similar behavior has been found for the TG gas in the harmonic trap [24]. Thus, the system of hard-core bosons mimics the macroscopic occupation of a momentum zero state and, in this aspect, resembles a uniform and non-interacting Bose system. The momentum distributions of non-commensurate case (fractional filling) are shown in Fig. 8 for various particle numbers. We can see that, in the fractional filling case, the profiles of momentum

distribution become narrower with the particle number increases, which is different from that in the commensurate case as we discussed before. This is because in this case, the system is a boson conductor, so the spatial distribution become more uniform with the particle number increases due to many body repulsions. The small oscillations in the momentum profiles come from finite size effects and it will vanish in the thermodynamic limit.

V. SUMMARY AND CONCLUSIONS

We have investigated the ground-state properties of a 1D TG gas in a periodic potential. Based on the exact many-body wave function, obtained from Bose-Fermi mapping theorem, we have calculated the SPRDM for considerable large system by employing the technique that the SPRDM can be expressed in a matrix product form in the TG gas limit. We calculated the occupation number of the lowest orbital by diagonalizing the SPRDM numerically. We found that fractional occupation of the lowest orbital decreases with particle number increases as $f_0 \propto 1/\ln(N)$ in the commensurate case while as $f_0 \propto 1/N^{0.44}$ in the non-commensurate case. So we conclude that there is no BEC for the TG gas in periodic potential in both the commensurate and the non-commensurate cases. We suspect that the scaling exponent of fractional occupations in the non-commensurate case may approach to 0.5 in thermodynamic limit. However, lack of data on bigger lattices prevented us to perform extensive finite size scaling analysis. We may seek analytic approaches to derive the observed scaling behavior of lowest orbital with particle number in the future. The momentum distributions of the TG gas show bosonic behavior and zero momentum peaks increase with the particle number as $n(0) \propto N$ at the commensurate case.

Acknowledgments

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